Linear Models 1

Machine Learning 2019
mlvu.github.io

machine learning: the basic recipe

Abstract your problem to a **standard task.**
Classification, **Regression**, Clustering, Density estimation, Generative Modeling, Online learning, Reinforcement Learning, Structured Output Learning

Choose your **instances** and their **features**.
For supervised learning, choose a target.

Choose your **model class**.
Linear models

Search for a good model.
Choose a **loss function**, choose a **search method** to minimise the loss.

Here is the basic recipe for the last lecture. Today we'll have a look at linear models, both for regression and classification. We'll see how to define a linear model, how to formulate a loss function and how to search for a model that minimises that loss function.

Most of the lecture will be focused on search method. The linear models themselves aren't that strong, but because they're pretty simple, we can use them to explain various search methods that we can also apply to more complex models

linear models and search

part 1:
Notation, defining the problem
Hyperplanes

Search
Random search, Evolutionary search

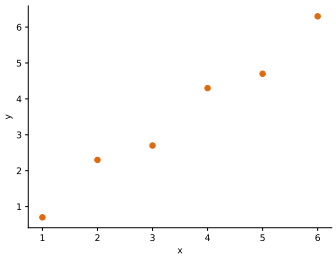
part 2:
Gradient Descent

Classification

The linear model in its basic form is pretty simple (and we've seen most of it already). So the thing we're going to focus on today is how to **search** for a good linear model. The search methods we'll discuss today are extremely versatile and form the basis for the majority of machine learning being done today (including all deep learning).

example data

x	y
1	0.7
2	2.3
3	2.7
4	4.3
5	4.7
6	6.3



We will start with **linear regression**, and use this dataset (with feature x and target variable y) as a running example.

We will assume that all our features are *numeric* for the time being.

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notation: one feature

$$X = x^1, x^2, x^3, \ldots$$
$$Y = y^1, y^2, y^3, \ldots$$

We will call the whole dataset (all instances) X. We will call the corresponding outputs Y.

Note that the superscript notation is slightly ambiguous, since it might also mean exponentiation. Hopefully, it will usually be clear from context which is intended.

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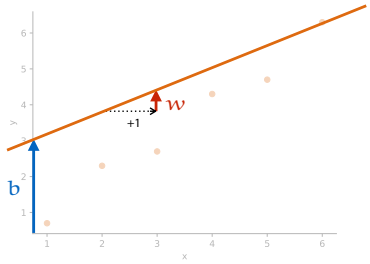
one feature

1 feature x: $f_{w,b}(x) = wx + b$



If we have one feature (as in this example) a standard linear regression model has two *parameters* (the numbers that determine which line we fit through our data): **w** the **weight** and **b**, the **bias**. The bias is also sometimes called the *intercept*.

b determines where the line crosses the vertical axis (or what value f takes when x = 0).

w determines how much the line rise if we move one step to the right (i.e. increase x by 1)

For the line drawn here, we have **b**=3 and **w** =0.5 (note that this isn't a very good fit for the data).

two features

1 feature x: $f_{w,b}(x) = wx + b$

2 features x_1, x_2:

$$f_{w_1,w_2,b}(x_1, x_2) = w_1x_1 + w_2x_2 + b$$

If we have two features, each feature gets its own **weight** (also known as a **coefficient**)

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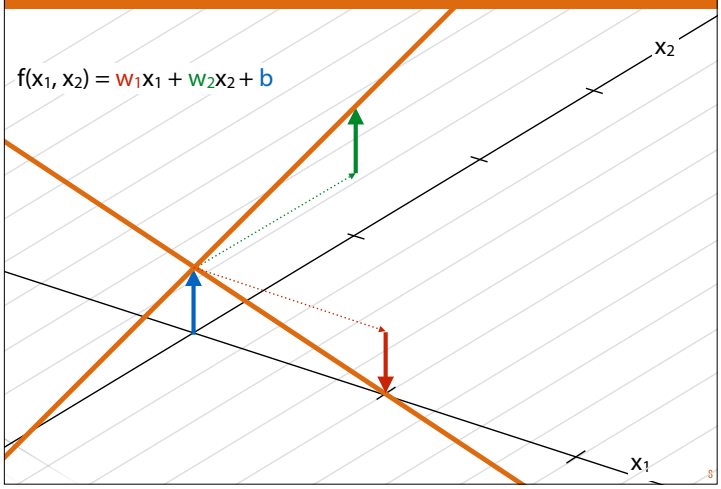
a 2D linear function



Here's what that looks like. The thick orange lines together indicate a plane (which rises in the x_2 direction, and declines in the x_1 direction). The parameter **b** describes how high above the origin this plane lies (what the value of f is if *both features* are 0). The value w_1 indicates how much f increases if we take a step of 1 along the x_1 axis, and the value w_2 indicates how much f increases if we take a step of size 1 along the x_2 axis.

---

multiple features

$$X = \mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^3, \ldots$$
$$Y = y^1, y^2, y^3, \ldots$$

$$\mathbf{x}^j = \begin{pmatrix} x_1^j \\ x_2^j \\ \vdots \\ x_m^j \end{pmatrix}$$ <- instance j, feature 1

In general, we would like to describe our algorithm for an arbitrary number of features, so that we can apply it to any dataset. To do this, we arrange the features of a single instance into a *vector*.

We will often omit the superscript j, in order to keep things legible.

for n features

$$f_{w,b}(x) = w_1 x_1 + w_2 x_2 + w_3 x_3 + \ldots + b$$

$$= w^T x + b$$

$$\text{with } w = \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} \text{ and } x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

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For an arbitrary number of features, it looks like this. We take the dot product of the data and the weights, and add a bias. The weights and the bias are the *parameters* of the model. We need to choose these to fit the model to our data.

We multiply each feature with its corresponding weight. This can be written as a *dot product* of two vectors.

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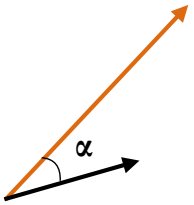
dot product

$$w^T x \quad \text{or} \quad w \cdot x$$

$$w^T x = \sum_i w_i x_i$$

$$= ||w||\ ||x|| \cos \alpha$$



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In this notation, we're using the **dot product**. The dot product of two vectors is simply the sum of the products of their elements. If we place the features into a vector and the weights, then a linear function is simply their dot product (plus the **b** parameter).

The transpose (superscript T) notation arises from the fact that if we make one vector a row vector and one a column vector, and matrix-multiply them, the result is the dot product (try it).

The dot product also has a geometric interpretation: the dot product is equal to the lengths of the two vectors, multiplied by the cosine of the angle between them. To get some intuition, review your Linear Algebra (or check **this link**).

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even more compact

$$f_w(x) = w^T x$$

$$\text{with } w = \begin{pmatrix} w_1 \\ \vdots \\ w_n \\ b \end{pmatrix} \text{ and } x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix}$$

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You can represent it even more compactly, by adding one more feature that you force to be always one. That way, you can add the **bias** to your weight vector.

There is a general principle at work here: we simplify our model (removing a term) but we keep the representational power by adding extra features. his is a very powerful principle, that we'll return to many times.

Usually, however, linear models are represented as in the previous slide: with an explicit, separate **bias**.

But which model fits our data best?

- loss function
- search method

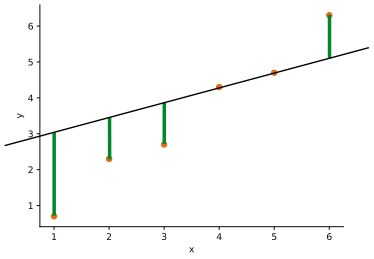
Given some data, which values should we choose for the parameter **w** and b?

In order to answer this question, we need two ingredients. First, we need a **loss function**, which tells us how well a particular choice of model does (for the given data) and second, we need a way to *search* the space of all models for a particular model that results in a low loss (a model for which the loss function returns a low value).

mean squared error loss

$$\text{loss}_{\mathbf{x},\mathbf{y}}(p) = \frac{1}{n}\sum_j \left(f_p(\mathbf{x}^j) - \mathbf{y}^j\right)^2$$

$$\text{loss}_{\mathbf{x},\mathbf{y}}(\mathbf{w}, b) = \frac{1}{n}\sum_j \left(\mathbf{w}^\top \mathbf{x}^j + b - \mathbf{y}^j\right)^2$$

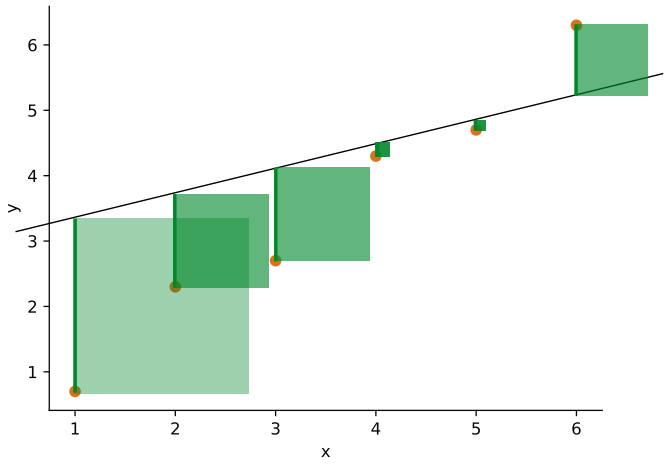


Here is a common loss function for regression: the mean-squared error (MSE) loss.

Note that the loss function takes a *model* as its argument. The model maps the data to the output, the loss function maps a model to a loss value. The data functions as a constant in the loss function.

It takes the residuals (differences between the model predictions and actual data), squares them, and returns the average (or the sum, sometimes). The square, as noted before, is mainly there to ensure that negative and positive residuals don't cancel out (giving us a small loss when we have big residuals).

It doesn't usually matter whether you divide by n (i.e. take the mean or the sum of the squares). Minimizing the sum is the same as minimising the mean (because n doesn't change)



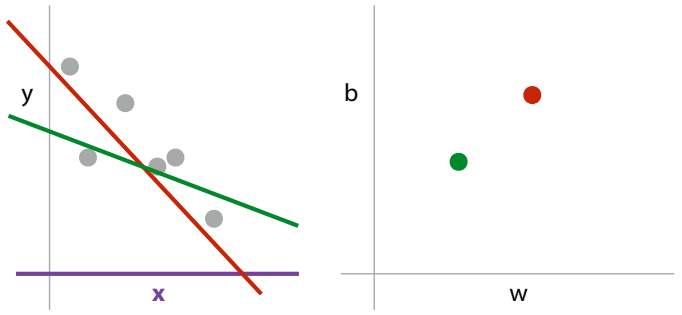
But the squares also have another effect. They ensure that the big errors affect the loss more heavily than small errors. You can visualise this as shown here: the mean squared error is the mean of the areas of the green squares (it's also called *sum-of-squares loss*).

When we search for a well-fitting model, the search will try to reduce the big squares much more than the small squares.

Other loss functions exist, and this is just a simple one to start with. In a later lecture, we will see that this loss function follows from the assumption that model is correct except for added noise from a *normal distribution*.

Visualization stolen from **https://machinelearningflashcards.com/**

model space



feature space
aka instance space

model space
aka hypothesis space

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Remember the two most important spaces of machine learning: the instance space and the model space. The loss function maps every point in the model space to a loss value. Here, the **instance space** is just the x axis.

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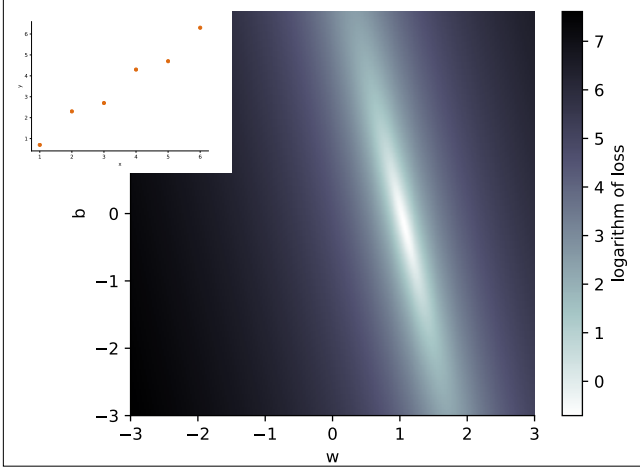
loss landscape



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As we saw in the previous lecture, we can plot the loss for every point in our model space. Here is what that actually looks like for the two parameters of the one-feature linear regression. Note that this is specific to the data we saw earlier. For a different dataset, we get a different loss landscape.

To minimize the loss, we need to search this space to find the brightest point in this picture. Remember that, normally, we have hundreds of parameters (one per feature) so it isn't as easy as it looks. Any method we come up with, needs to work in any number of dimensions.

We've plotted the logarithm of the loss as a trick to make this image visually easier to understand (it maps the values that are easy to tell apart to the values we care about). The logarithm is a monotonic function so log(loss(w, b)) has its minimum at the same place as loss(w, b).

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optimization

$$\hat{p} = \arg\min_{p} \text{loss}_{X,Y}(p)$$

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The mathematical name for this sort of search is **optimization**. That is, we are trying to find the input (the model parameters) for which a particular function (the loss) is at its optimum (a maximum or minimum, in this case a minimum). Failing that, we'd like to find as low a value as possible.

random search

start with a random point **p** in the model space

loop:

pick a random point **p′** close to **p**

if loss(**p′**) < loss(**p**):

p <- **p′**

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Let's start with a very simple example: random search.

To implement this we need to define what exactly we mean by "close to".

analogy: hiker in a snowstorm

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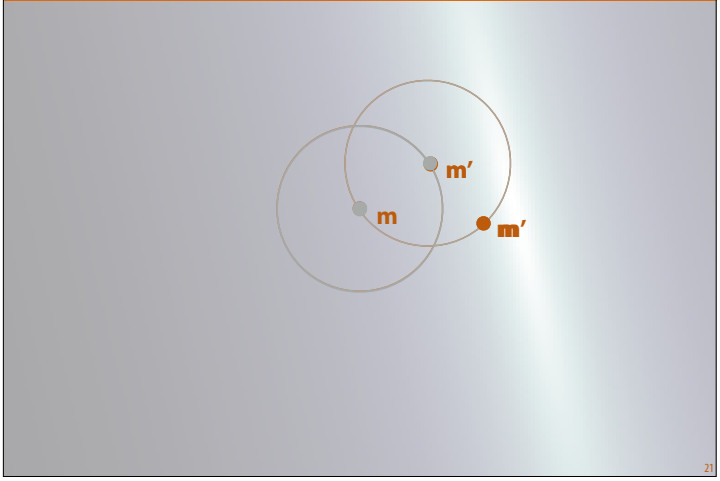
A common analogy is a *hiker in a snowstorm*. Imagine you're hiking in the mountains, and you're caught in a snowstorm. You can't see a thing, and you'd like to get down to your hotel in the valley, or failing that, you'd like to get to as low a point as possible.

You take a couple of steps in every direction to see in which direction the mountain goes down quickest. You take a big step in that direction, and then repeat the process. This is, in effect, what random search is doing. More importantly, it's how blind random search is to the larger structure of the landscape.

image source: ***https://www.wbur.org/hereandnow/2016/12/19/rescue-algonquin-mountain***

"close to"



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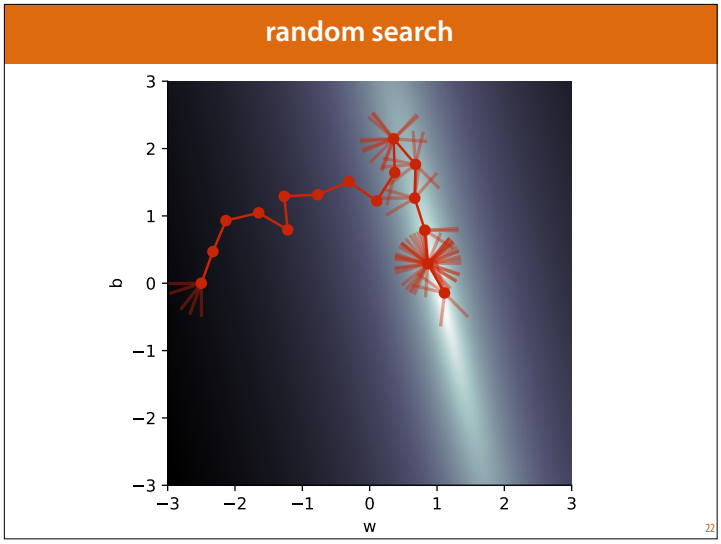
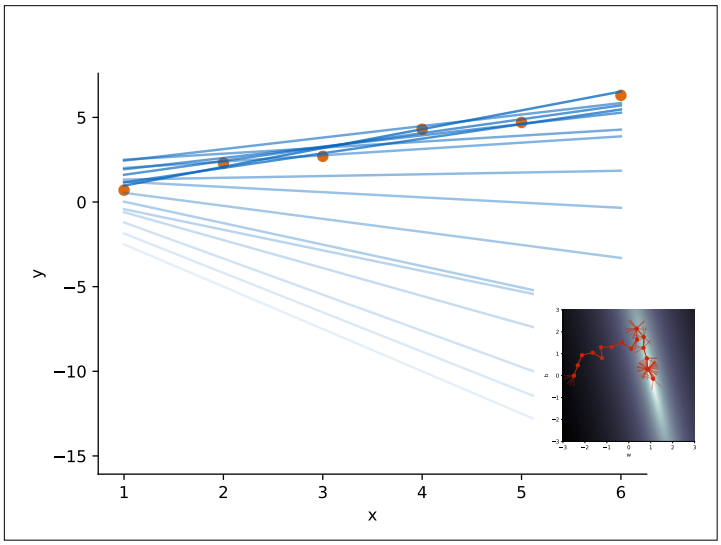
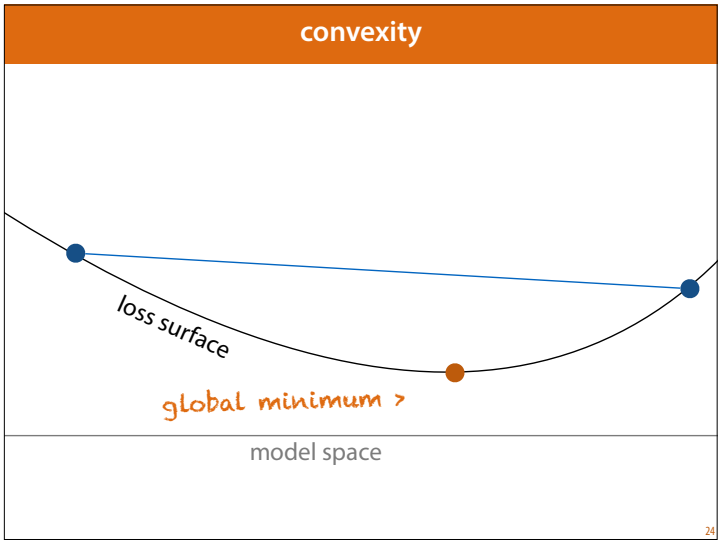
The basic random search algorithm chooses the next point by sampling uniformly among all points with some pre-chosen distance r from w. Formally: it picks from the hypersphere (or circle, in 2D) with radius r, centered on **w**.



Here is random search in action. The transparent red offshoots are successors that turned out to be worse than the current point. The algorithm starts on the left, and slowly (with a bit of a detour) stumbles in the direction of the low loss region.



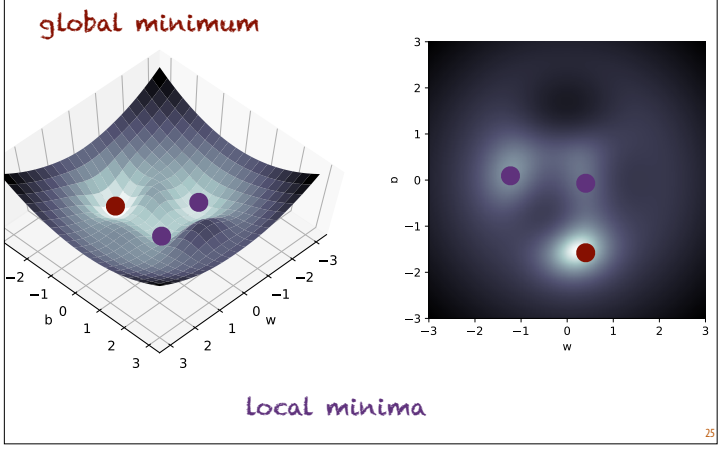
Here is what it looks like in **feature space**. The first model (bottom-most line) is entirely wrong, and the search slowly moves, step by step, towards a reasonable fit on the data.



One of the reasons such a simple approach works well enough for our problem is that our problem is **convex**. A surface (like our loss landscape) is convex if a line drawn between any two points on the surface lies entirely above the surface. One of the implications of convexity is that there is only one minimum.

This minimum is the optimal model. So long as we know we're moving down (to a point with lower loss), we can be sure we're moving in the direction of the minimum.

local vs global minima



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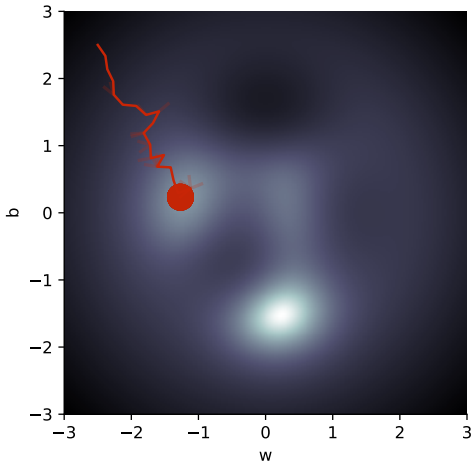
So let's look at what happens if the loss surface isn't convex: what if the loss surface has multiple *local minima*?

Here's a loss surface (not based on an actual model with data, just some function) with a more complex structure. The two purple points are the lowest point in their respective *neighborhoods*, but the red point is the lowest point globally.



Here we see random search on our more complex loss surface. As you can see, it makes a beeline for one of the local minima, and then gets stuck there. No matter how many more iterations we give it, it will never escape.

Note that changing the step size will not help us here. Once the search is stuck, it stays stuck.

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simulated annealing

pick a random point **p** in the model space

loop:

  pick a random point **p'** close to **p**

  if loss(**p'**) < loss(**p**):

    p <- **p'**

  else:

    with probability q: **p** <- **p'**

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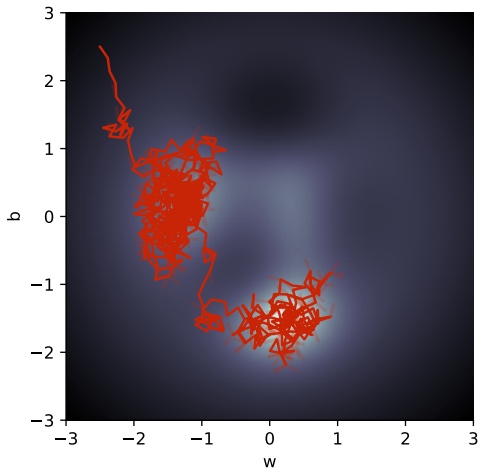
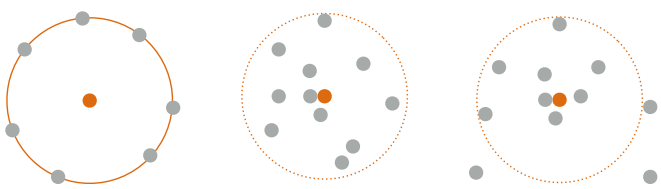
Here's a simple trick that can help us escape local minima: if the next point chosen isn't better than the current one, we still pick it, but only with some small probability. In other words, we allow the algorithm to *occasionally* travel uphill. This means that whenever it gets stuck in a local minimum, it still has some probability of escaping, and finding the global minimum.



Here is a run of simulated annealing. Of course, with SA there is always the possibility that it will jump out of the global minimum again and move to a worse minimum. That shouldn't worry us, however, so long as we remember the best model we've observed. Then we can just let SA jump around the model space driven partly by random noise, and partly by the loss surface.

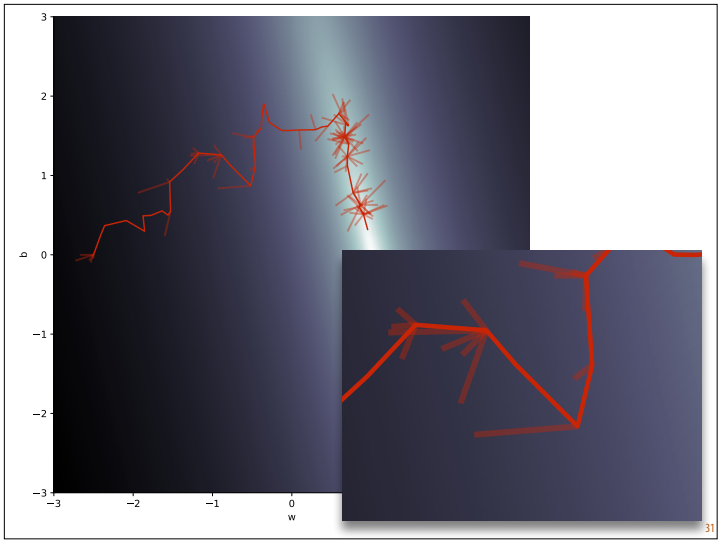
Note: in many situations, the local minima are fine. We do not always need an algorithm that is guaranteed to find the global minimum.

Variations



Fixed radius | Random uniform | Normal

The fixed step size we used so far is just one way to sample the next point. To allow the algorithm to occasionally make smaller steps, you can sample m' so that it is *at most* some distance away from m, instead of *exactly*. Another approach is to sample the distance from **a Normal distribution**. That way, most points will be close to the original m, but every point in the model space can theoretically be reached in one step.



Here is what random search looks when the steps are sampled from a normal distribution. Note that the "failed" steps all have different sizes.

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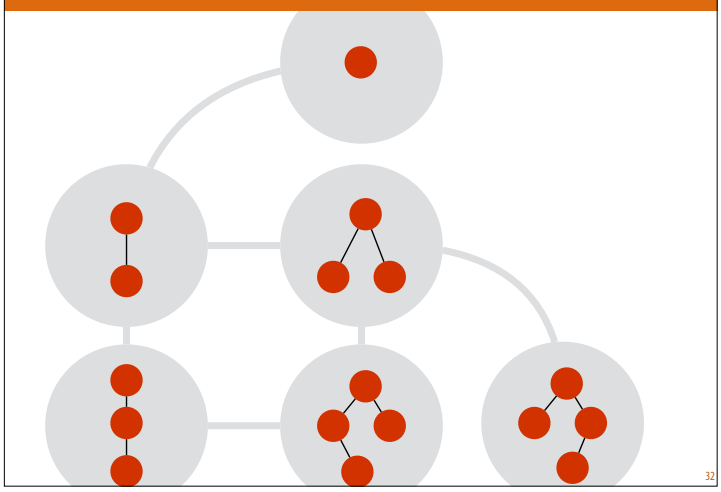
discrete model spaces



The space of linear models is *continuous*: between every two models, there is always another model, no matter how close they are together. * If your model space is discrete, for instance in the case of tree models, you can still apply random search and simulated annealing. You just need to define which models are "close" to each other. Here we say that two trees are close if I can turn one into the other by adding or removing a single node.

Random search and SA can now be used to search this graph to find the tree model that gives the best performance. Note that in practice, we usually use a different model to search for decision trees and regression trees. We will introduce this algorithm in a later lecture.

* Strictly speaking this is not a correct definition of a continuous space. It suffices for our purposes.

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black box optimization

random search, simulated annealing:

- very simple
- we only need to compute the loss function for each model
- can require many iterations
- also works for discrete model spaces (like tree models)

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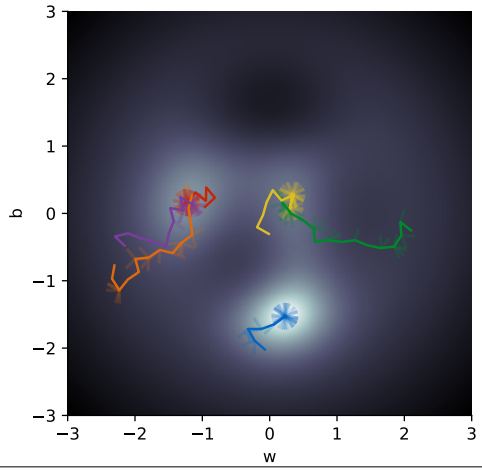
Black box optimization refers to those optimisation methods that only require us to be able to compute the loss function. We don;don't need to know anything about the model, or the domain.

parallel search



Another thing you can do is just to run random search a couple of times independently (one after the other, or in parallel). If you're lucky one of these runs may start you off close enough to the global minimum.

For simulated annealing, doing multiple runs makes less sense. There's not much difference between 10 runs of 100 iterations and one run of 1000. The only reason to do multiple runs of SA is because it's easier to parallelize over multiple cores or machines.

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population methods

evolutionary algorithms (genetic algorithms evolutionary strategies, etc)

particle swarm optimization

ant colony optimization

To make parallel search even more useful, we can introduce some form of communication between the searches happening in parallel. If we see the parallel searches as a population of agents that occasionally "communicate", we can guide the search a lot more. Here are some examples. we won't go into this too deeply. We will only take a (very) brief look at evolutionary methods.

Often, there are specific variants for discrete and for continuous model spaces.

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evolutionary algorithms

Start with a *population* of k models.

loop:

rank the population by loss

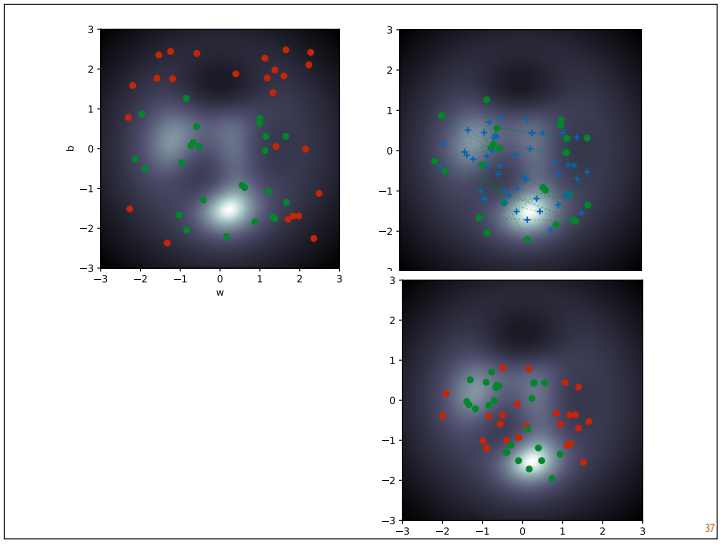
remove the half with the worst loss

"breed" a new population of k models

optional: add a little noise to each child.

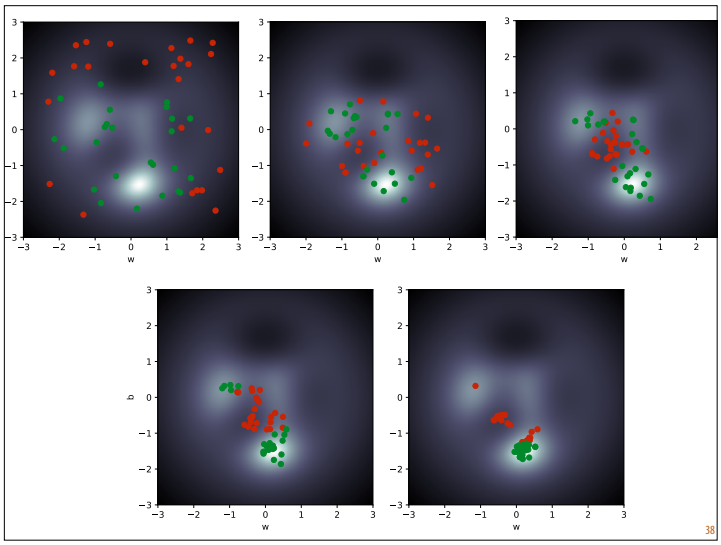
Here is a basic outline of an evolutionary method (although many variations exist). In order to instantiate this, we need to define what it means to "breed" a population of new models from an existing population. A common approach is to select to random parents and to somehow average their models. This is easy to do in a continuous model space (we can literally average the two parent models to create a child). In a discrete model space, it's more difficult, and it depends on the specifics of the model space.

The breeding process (sometimes called the **crossover operator**) is usually the most difficult part of designing an evolutionary algorithm.



Here's what that looks like. We start with a population of 50 models, and compute the loss for each. We kill the worst 50% (the red dots) and keep the best 50%. We then create a new population (the blue crosses), by randomly pairing up parents from the green population, and taking the point halfway between the two parents, with a little noise added.

We then take the blue crosses as the new population and iterate.



Here are five iterations of the algorithm. Note that in the intermediate stages, the population covers both the local and the global minima.

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population methods

Powerful

Black box

Easy to parallelise

Slow/expensive for complex models

Difficult to tune

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To make parallel search even more useful, we can introduce some form of communication between the searches happening in parallel. If we see the parallel searches as a population of agents that occasionally "communicate", we can guide the search a lot more. Here are some examples. we won't go into this too deeply. We will only take a (very) brief look at evolutionary methods.

Often, there are specific variants for discrete and for continuous model spaces.

towards gradient descent: branching search

pick a random point **p** in the model space

loop:

pick **k** random points {$\mathbf{p}_i$} close to **p**

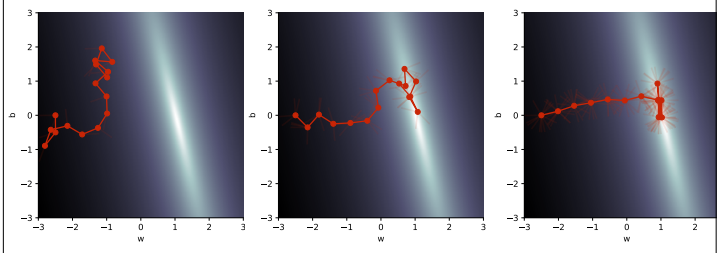
p' <- $\text{argmin}_{\mathbf{p}_i}$ loss($\mathbf{p}_i$)

if loss(**p'**) < loss(**p**):

p <- **p'**

Finally, as a bridge to what we'll discuss after the break: here is another, simple variation, which I've called branching search (I couldn't find an official name).

k=2 k=5 k=15



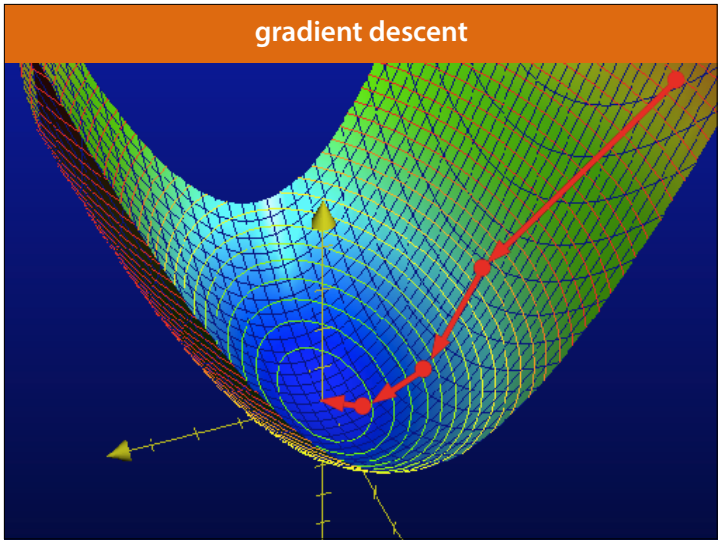
As you can see, the more samples we take, the more directly we head for the region of low loss. The more closely we inspect our local neighbourhood, to determine in which direction the function decreases quickest, the faster we converge.

To escape local minima:

- add randomness, add multiple models

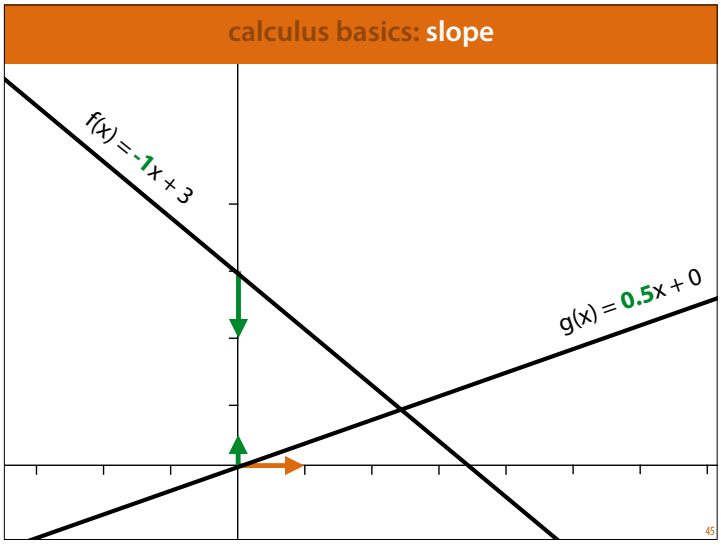
To converge faster:

- combine known good models (breeding)
- **inspect the local neighbourhood**



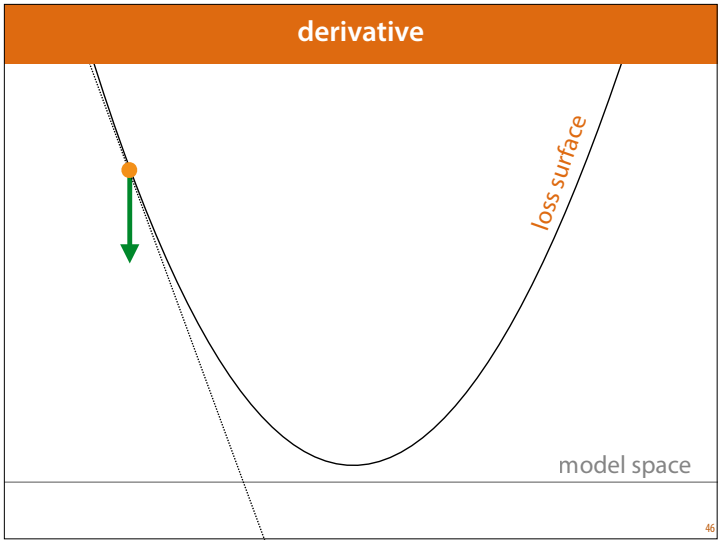
However, if our model space is continuous, and if our loss function is smooth, we don't *need* to take multiple samples to guess the direction of fastest descent: we can simply derive it, using calculus. This is the basis of the **gradient descent algorithm**, which we will discuss after the break.

image source: **http://charlesfranzen.com/posts/multiple-regression-in-python-gradient-descent/**



Before we dig in to the gradient descent algorithm, let's review some basic principles from calculus. First up, *slope*. The slope of a linear function is simply **how much it moves up** if **we move one step to the right**. In the case of f(x) in this picture, the slope is *negative*, because the line moves down.

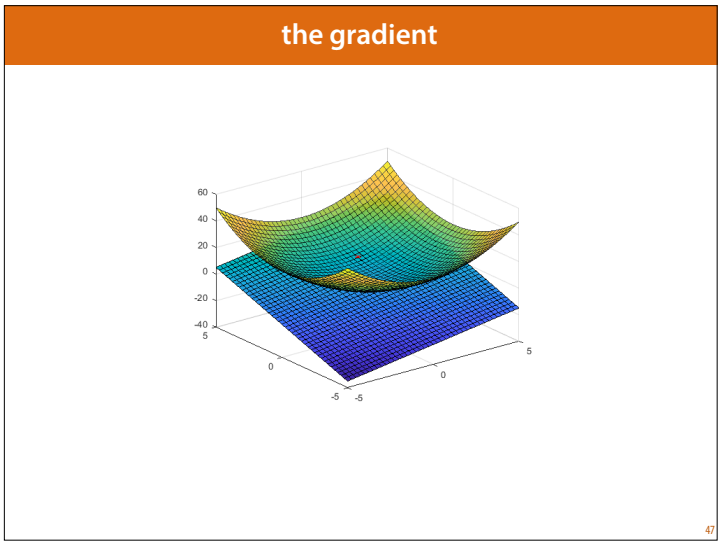
In our regression model, the parameter w was the slope.



The **tangent line** of a function at particular point **x** is the line that just touches the function at **x**. The **derivative of the function gives us the slope of the tangent line**. Traditionally we find the minimum of a function by setting the derivative equal to 0 and solving for **x** (giving us the point where the tangent is a horizontal line).

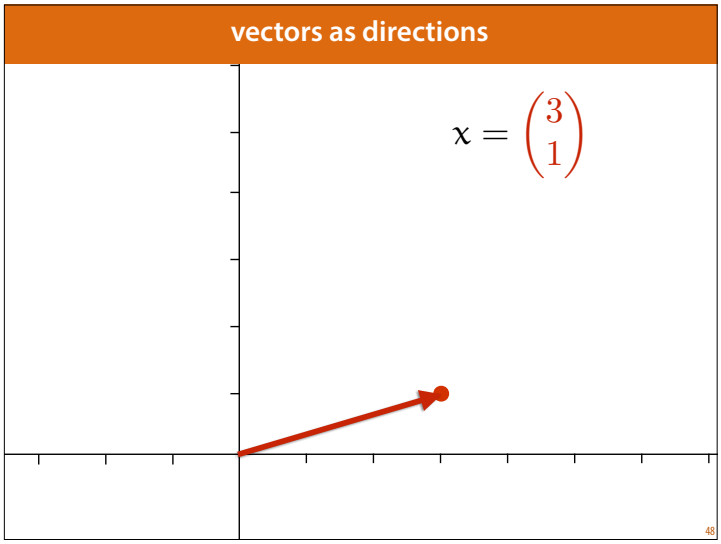
For complex models, it may not be possible to solve for x, but we can still use the gradient to *search* for the minimum. Looking at the example above, we note that the tangent line moves down (i.e. the slope is negative). This tells us that we should move to the right to follow the function downward. As we take small steps to the right, the derivative stays negative, but gets smaller and smaller as we close in on the minimum. This suggests that the *magnitude* of the slope lets us know how big the steps are that we should take, and the *sign* gives us the direction.

A useful analogy is to think of putting a marble at some point on the curve and following it as it rolls downhill to find the lowest point.



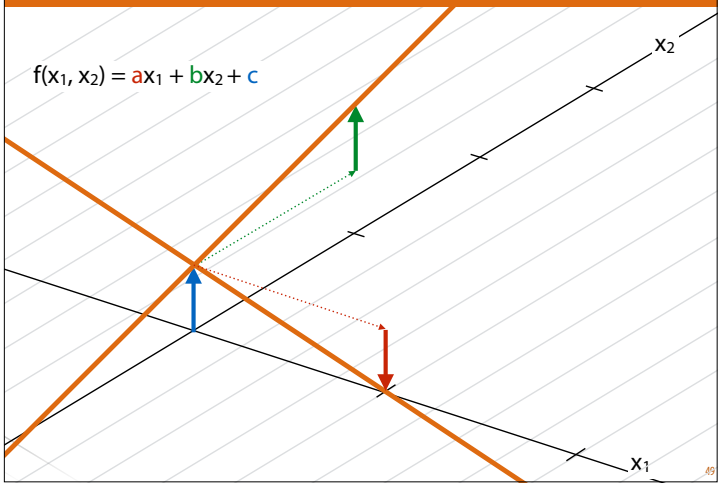
To apply this principle to machine learning, we'll need to generalise it for loss functions with multiple inputs (i.e. models with multiple parameters). We do this by generalising the *derivative* to the ***gradient***. The tangent line becomes a tangent (hyper)plane. The hyperplane will gives us both a direction to move in, and an indication of how big a step we should take in that direction.

image source: **https://nl.mathworks.com/help/matlab/math/calculate-tangent-plane-to-surface.html?requestedDomain=true**



To properly explain the details, we need to look at a few basics. First, we're used to thinking of vectors as points in the plane. But they can also be used to represent *directions*. In this case we use the vector to represent the arrow from the origin to the point. This gives us a direction (the direction in which the arrow points), and a magnitude (the length of the arrow).

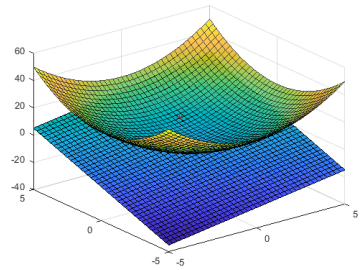
a 2D linear function



Returning to the subject of slopes: the two weights of a linear 2D function (a and b) representing a hyperplane, are just one slope per dimension. If we move one step in the direction of x_1, we move up by a, and if we move one step in the direction of x_2, we move up by b.

gradient

$$\nabla f(x, y, z) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)$$

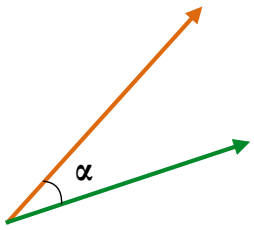


We are now ready to define the gradient. Any function from n inputs to one output has n variables for which we can take the derivative. These are called partial derivatives: they work the same way as regular derivatives, except that you when you take the derivative with respect to one variable x, you treat the other variables as constants. For technical reasons, the derivative is *row* vector, not a column vector.

If a particular function f(x) has gradient w for input x, then g(**x**) = $\mathbf{w}^T\mathbf{x}$ + b (for some b) is the tangent hyperplane at **x**.

w: direction of steepest ascent

$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$
$$= ||\mathbf{w}||\ ||\mathbf{x}|| \cos(\alpha)$$



So let's assume we have some plane , described by function g(x) = $\mathbf{w}^T\mathbf{x}$ + b, that *just* touches our loss function. Which direction is the direction of steepest ascent? In which direction does the function g(x) increase quickest?

Since g is linear, many details don't matter: we can set b to zero, since that just translates the hyperplane up or down. It doesn't matter *how big* a step we take in any direction, so we'll take a step of size 1. Finally, it doesn't matter where we start from, so we will just start from the origin. So the question becomes: for which input of magnitude 1 does g provide the biggest output?

To see the answer, we need to use the geometric interpretation of the dot product. Since we required that ||**x**||= 1, this disappears from the equation, and we only need to maximise the quantity ||**w**|| cos(α) (where only α depends on our choice of input, **w** is given). cos(α) is maximal when α is zero: that is, when **x** and **w** are pointing in the same direction.

In short: w, the gradient, *is* the direction of steepest ascent on the plane.

gradient descent

pick a random point **m** in the model space

loop:

m ← **m** - η ∇loss(**m**)

we usually set η somewhere between 0.0001 and 0.1

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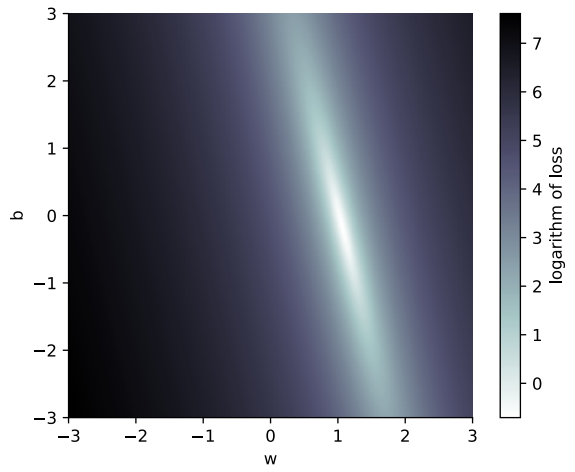
Here is the gradient descent algorithm. Starting from some candidate **m**, we simply compute the gradient at **m**, subtract it from the current choice, and iterate this process.

- We *subtract*, because the gradient points *uphill*. Since the gradient is the direction of steepest ascent, the negative gradient is the direction of steepest *de*scent.
- Since the gradient is only a *linear approximation* to our loss function, the bigger our step the bigger the approximation error. Usually we scale down the step size indicated by the gradient by multiplying it by a learning rate η. This value is chosen by trial and error, and remains constant throughout the search.

Note a potential point of confusion: we have two linear functions here. One is the *model*, whose parameters are indicated by **w** and b. The other is the tangent hyperplane to the loss function, whose slope is indicated by ∇loss(**m**) here (but by **w** in the previous slide). These are different functions on different spaces.



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Let's go back to our example problem, and see how we can apply gradient descent here.

$$\text{loss}(w, b) = \frac{1}{n} \sum_j (wx^j + b - y^j)^2$$

$$\nabla \text{loss}(w, b) = \left(\frac{\partial \text{loss}(w, b)}{\partial w}, \frac{\partial \text{loss}(w, b)}{\partial b} \right)$$

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Here is our loss function again, and the two partial derivatives we need work out to find the gradient.

$$\frac{\partial \text{loss}(w, b)}{\partial w} = \frac{\partial \frac{1}{n}\sum_i (wx_i + b - y_i)^2}{\partial w}$$
$$= \frac{1}{n}\sum_i \frac{\partial (wx_i + b - y_i)^2}{\partial w}$$
$$= \frac{1}{n}\sum_i \frac{\partial (wx_i + b - y_i)^2}{\partial (wx_i + b - y_i)} \frac{\partial (wx_i + b - y_i)}{\partial w}$$
$$= \frac{2}{n}\sum_i (wx_i + b - y_i)x_i$$

$$\frac{\partial \text{loss}(w, b)}{\partial s} = \frac{\partial \frac{1}{n}\sum_i (wx_i + b - y_i)^2}{\partial b}$$
$$= \frac{2}{n}\sum_i (wx_i + b - y_i)$$

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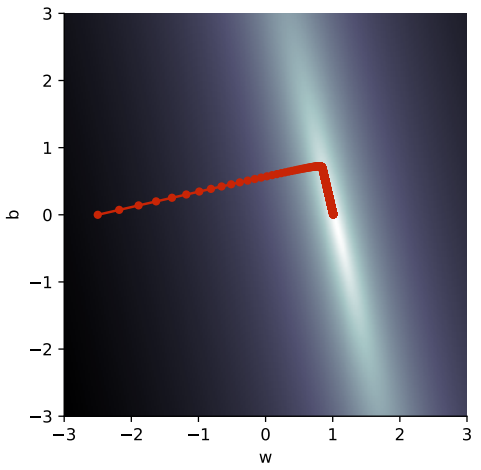
Here are the derivations of the two partial derivatives:

- first we use the *sum rule*, moving the derivative inside the sum symbol
- then we use the *chain rule*, to split the function into the composition of computing the residual and squaring, computing the derivative of each with respect to its argument.

The second homework exercise provides a list of the most common rules for derivatives.



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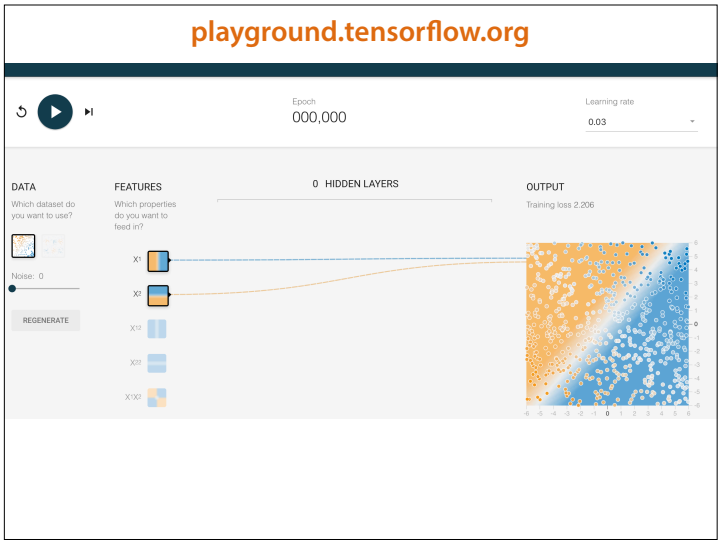
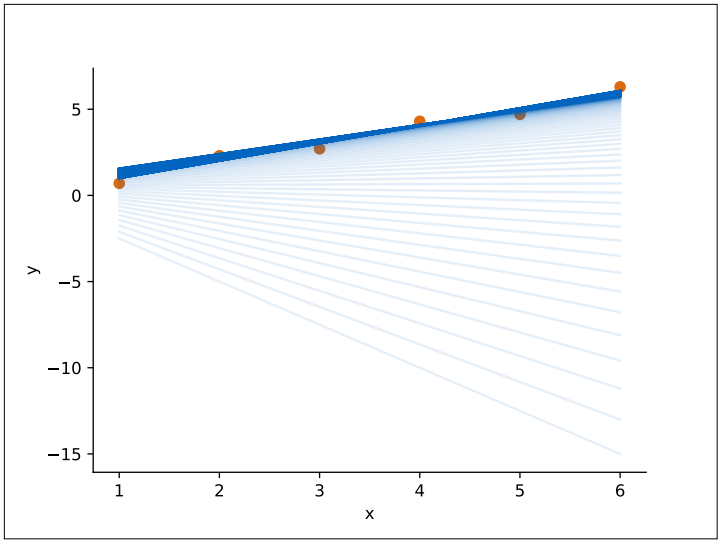
Here is the result. Note how the iteration converges directly to the minimum. Note also that we have no rejections: the algorithm is fully deterministic: it computes the optimal step, and takes it.

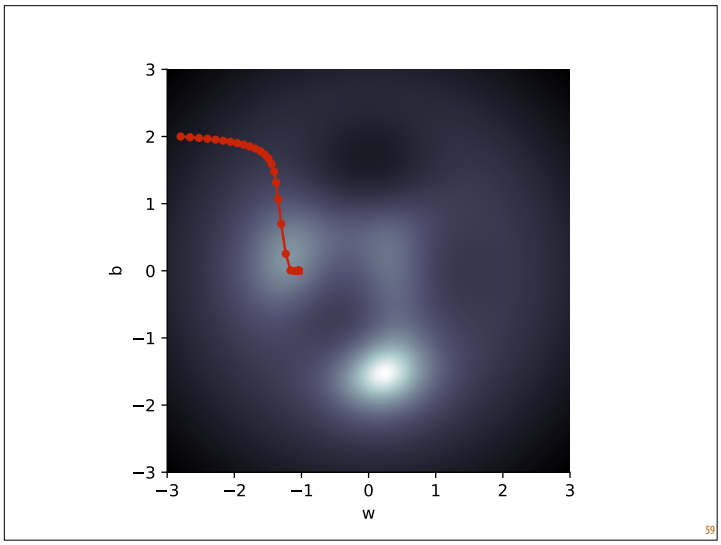


Here is a very helpful little browser app that we'll return to a few times during the course. If you click the image, you'll see the stripped down version that lets you play with gradient descent on a regression problem with two features. Tthe output for the data is indicated by the color of the points, the output of the model is indicated by the colouring of the plane.

Note that the page calls this model a neural network (which we won't discuss for a few more weeks). You can see linear models like these as very simple neural networks.

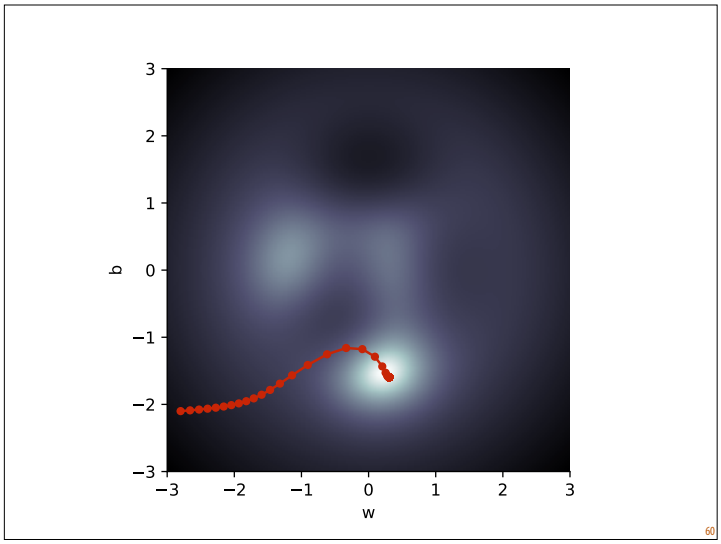


Here is what it looks like in feature space.



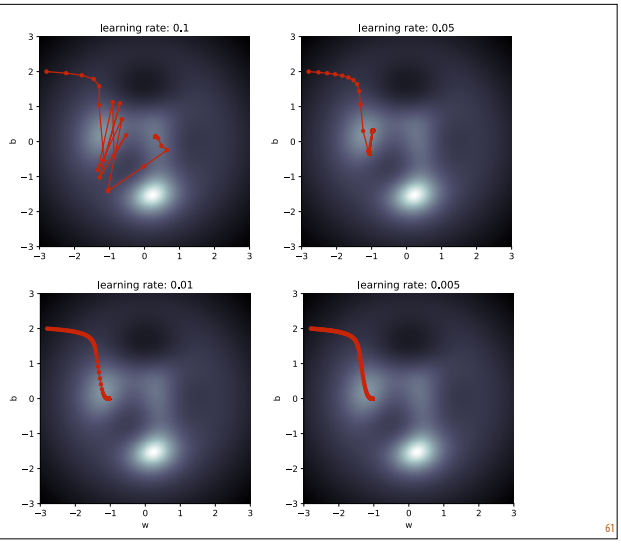
If our function is non-convex, gradient descent doesn't help us with local minima. As we see here, it heads straight for the nearest minimum and stays there. To make the algorithm more robust against this type of thing, we need to add a little randomness back in, preferably without destroying the behaviour of moving so cleanly to a minimum once one is found.

We can try multiple starting points. Later we will see *stochastic* gradient descent, which computes the gradient only over subsets of the data (making the algorithm more efficient, and adding a little randomness at the same time).



Here is a more fortunate run.

NB: The point of convergence seems a little off in these images. The partial derivatives for this function are very complex (I used **Wolfram Alpha** to find them). Most likely, the implementation causes some numerical instability.



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but actually…

$$\frac{\partial \text{loss}(w, b)}{\partial w} = 0$$

$$\frac{\partial \text{loss}(w, b)}{\partial b} = 0$$

there's an analytical solution (for this model)

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It's worth saying that for linear regression, although it makes a nice, simple illustration, none of this is actually necessary. For linear regression, we can set the derivatives equal to zero and solve explicitly for **w** and for **b**. For many other models, however, we are not so lucky, and search is required.

gradient descent

only works for continuous model spaces

… with smooth loss functions

… for which we can work out the gradient

does not escape local minima

very fast, low memory

very accurate

backbone of 99% of modern machine learning.

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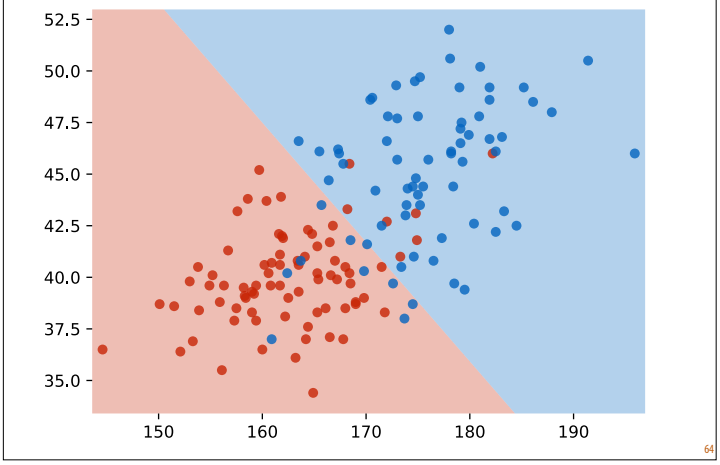
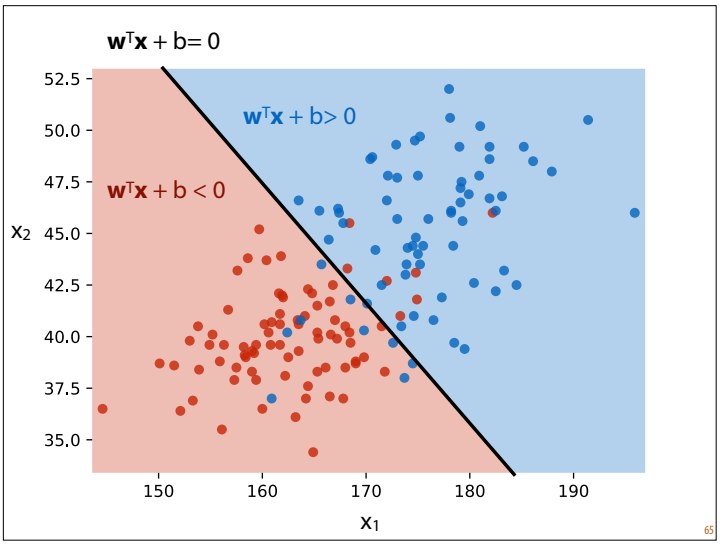
classification

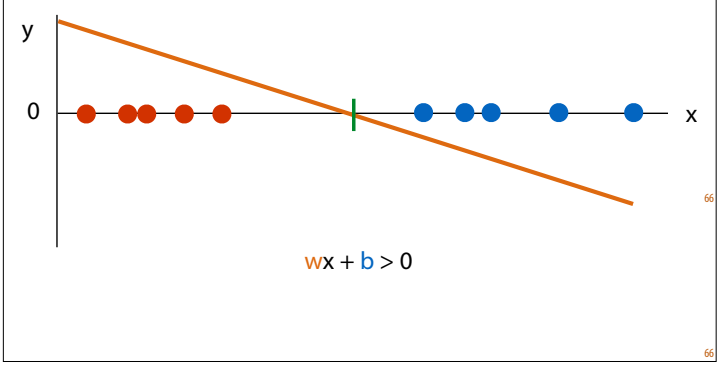


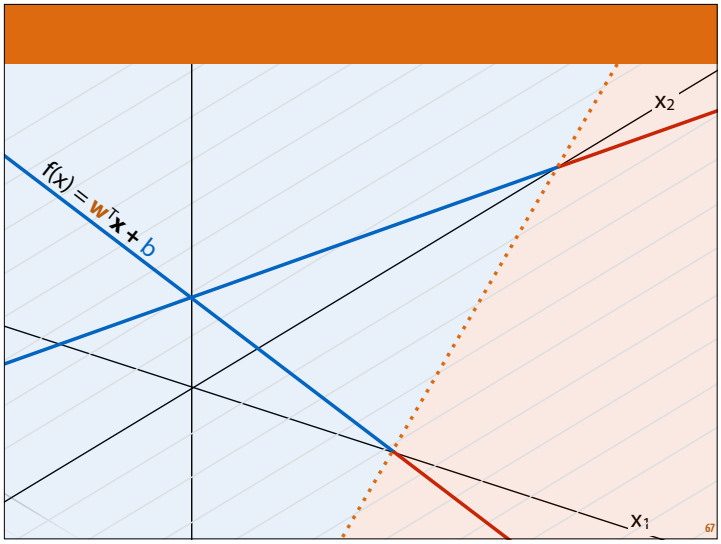
Now, let's look at how this works for classification. How do we define a linear classifier: that is a classifier whose decision boundary is always a line in instance space.



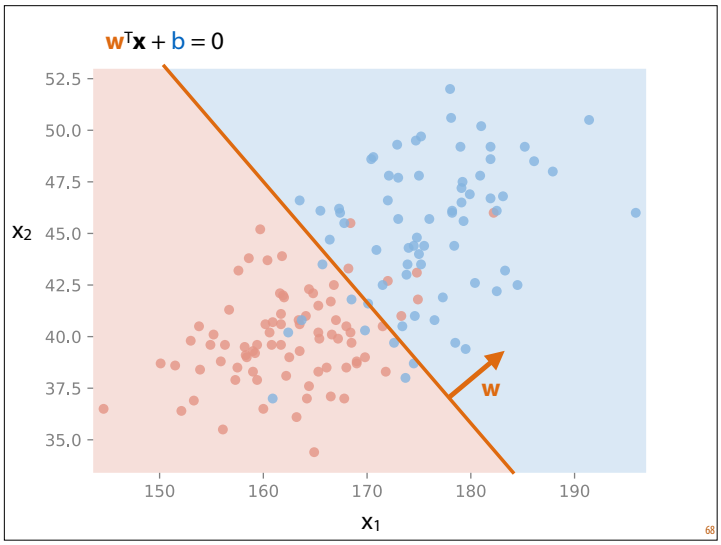
To define a linear decision boundary, we take the same functional form: some weight vector **w**, and a bias b. If $\mathbf{w}^T\mathbf{x} + b$ is larger than 0, we call **x** one class, if it is smaller than 0, we call it the other (we'll stick to binary classification for now).

1D linear classifier





The function f(x) = $\mathbf{w}^T\mathbf{x}$ + b describes a linear function from our feature space to a single value. Here it is in 2D: a plane that intersects the feature space. The line of intersection is our decision boundary.

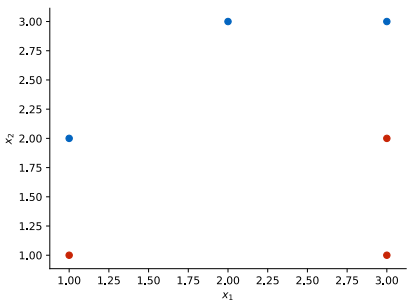


This also shows us how to interpret **w**. Since it is the direction of steepest ascent, it is the vector **perpendicular to the decision boundary**, pointing to the class we assigned to the case where $\mathbf{w}^T\mathbf{x}$ + b is larger than 0 (the blue class in this case).

---

example data

x_1	x_2	
1	2	true
1	1	false
2	3	true
3	3	true
3	1	false
3	2	false



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Here is a simple classification dataset, which we'll use to illustrate the principle.

loss?

nr. of misclassified examples (error)?

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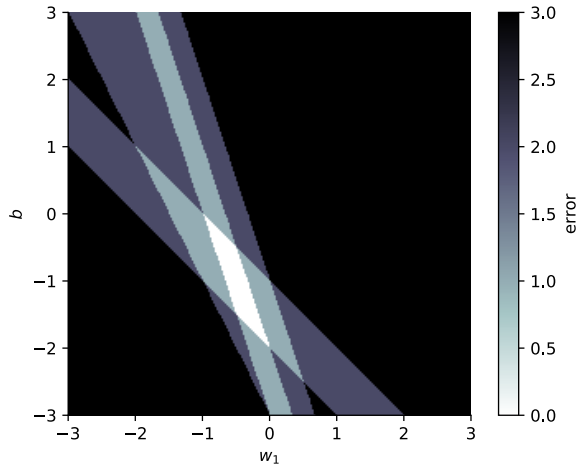
This gives us a model space, but how do we decide the quality of any particular model? What is our **loss function** for classification?

The thing we are (usually) trying to minimise is the **error**: the number of misclassified examples.



This is what our loss surface looks like for that loss function. Note that it consists almost entirely of flat regions. This is because changing a model a tiny bit will usually not change the number of misclassified examples. And if it does, the loss function will suddenly jump a lot.

In these regions, random search would have to do a random walk, stumbling around until it finds a ridge by accident.

Gradient descent would fare even worse: the gradient is zero everywhere in this picture (except exactly on the ridges, where it is undefined).

Note that our model now has three parameters w_1, w_2 and b. In order to plot the loss surface in two dimensions, we have fixed w_2=1.

Sometimes your loss function should not be the same as your evaluation function.

This is an important lesson about loss functions. They serve two purposes:

1. to express what quality we want to maximise in our search for a good model
2. to provide a smooth loss surface, so that we can find a path from a bad model to a good one

For this reason, it's common not to use the error as a loss function, even though it's the thing we're actually interested in minimizing. We'd like to replace it by a loss function that has its minimum at (roughly) the same model, but that provides a smooth loss surface.

classification losses

Least squares loss (today)

Log loss / logistic regression (week 3, Probability 1)

SVM loss (week 3, Linear Models 2)

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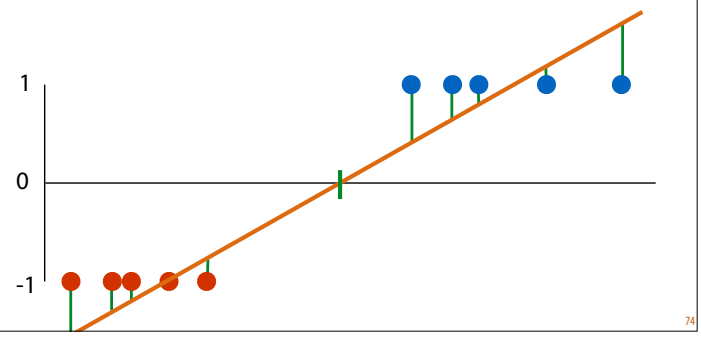
In this course, we will investigate three common loss functions for classification. The first, least-squares loss, is just an application of MSE loss to classification, we will discuss that in the remainder of the lecture. The others require a bit more background. We will discuss these in week three.

---

least-squares loss

$$\text{loss}(\mathbf{w}, b) = \sum_{i \in \text{pos}} (\mathbf{w}^T \mathbf{x}_i + b - 1)^2 + \sum_{i \in \text{neg}} (\mathbf{w}^T \mathbf{x}_i + b + 1)^2$$



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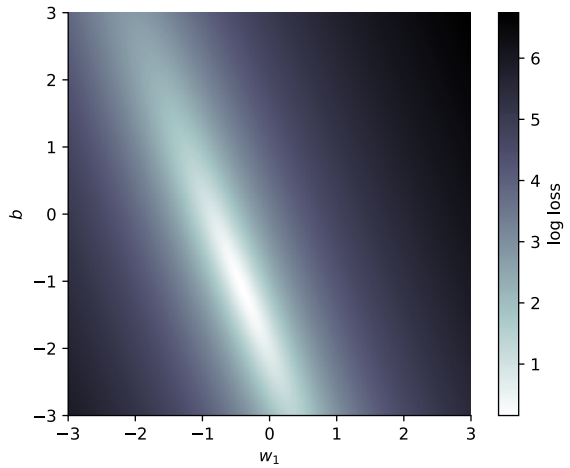
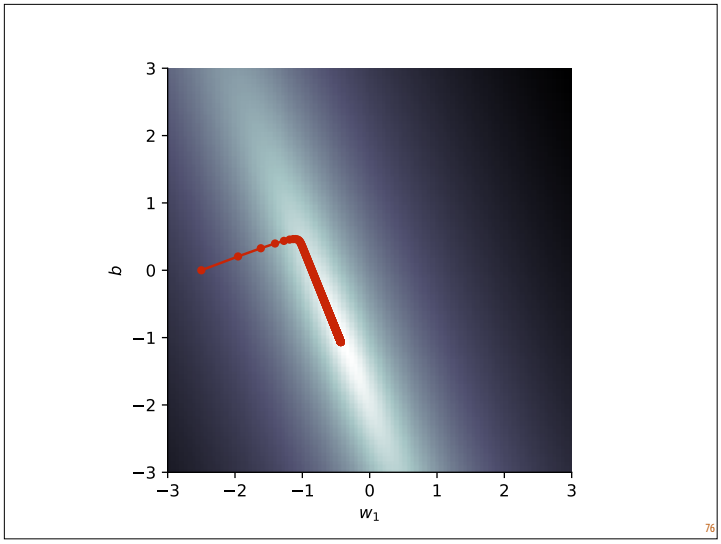
There are a few loss functions available for classification. We'll give you a simple one now, the least squares loss for classification, and come back to this problem later.

The least squares classifier essentially turns the classification into a regression problem: it assigns positive points the numeric value +1 and negative points the value -1, we then use a basic MSE loss that we saw before the break. Since we are look for a linear function that is positive for point in the positive class and negative for points in the negative class, this is a reasonable approach.

Performing gradient descent with this loss function will result in a line that minimised the green residuals. Hopefully the points are far apart that the decision boundary(the **single point** where the orange line crosses the x axis) separates the two classes.

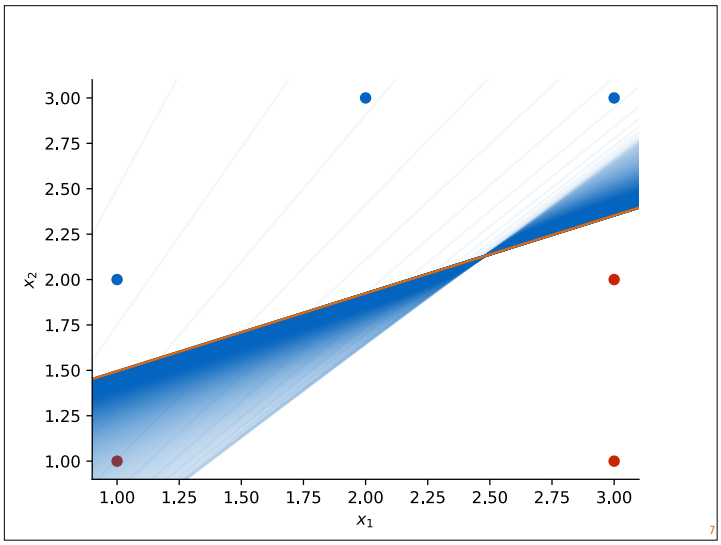


With this loss function, we note that our loss surface is perfectly smooth.

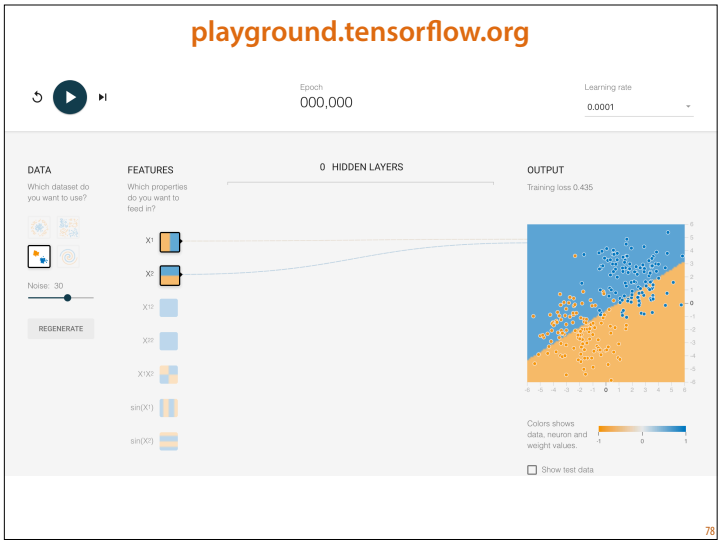


And gradient descent has no problem finding a solution.

Note, however that the optimum under this loss function may not perfectly separate the classes, even if they *are* linearly separable. We'll see some other loss functions later that provide a better optimum as well as a smooth loss surface.



Here is the result in instance space, with the final decision boundary in orange.



The tensor flow playground also allows us to play around with linear classifiers. Note that only for one of the two classifiers, the linear decision boundary is appropriate.

This example actually uses a logistic regression loss, rather than a least squares loss. We'll discuss logistic regression (which, confusingly, is a classification method) in the first probability lecture.

summary

Black box optimization:
- Random search, Simulated Annealing, Evolutionary
- Simple, works on discrete model spaces

Gradient descent:
- Powerful, only on continuous model spaces
- Very important, will see again

For classification:
- Find a smooth loss function
- least squares loss (more on this later)

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